WHAT IS CLAIMED IS:

1 A method of identifying drug non-target biomolecules in a mixture of biomolecules, comprising:

interacting mixture of biomolecules with a collection of capture compounds, wherein the collection comprises a plurality of capture compounds, comprising sets of capture compounds, wherein each set of capture compounds includes a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomlecules when the selectivity moiety is present than in its absence; and a moiety Z for presenting X and Y; and

analyzing the captured biomolecules to identify drug non-targets.

2. A method of identifying drug non-target biomolecules in a mixture of biomolecules, comprising:

interacting mixture of biomolecules with a capture compound, wherein the capture compound includes a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomlecules when the selectivity moiety is present than in its absence; and a moiety Z for presenting X and Y; and

analyzing the captured biomolecules to identify drug non-target.

3. The method of claim 1 wherein, each set of capture compounds further includes a moiety Q on the moiety Z, such that each set contains a different Q, wherein Q permits separation of each set.

4. The method of claim 1 wherein, the moiety Y is a pharmaceutical drug, drug fragment, drug metabolite or prodrug.

5. The method of claim 1 wherein, the moiety Y is linked to the

moiety Z in different orientations via different points of attachments on the moiety

6. The method of claim 1, wherein the biomolecules are proteins.

7. The method of claim 1, wherein the biomolecules are receptors.

8. The method of claim 1, wherein the biomolecules are liver enzymes.

9. The method of claim 1, wherein the biomolecules are enzymes.

10. The method of claim 1, wherein Q permits separation of capture compounds by arraying of the capture compounds on a solid support by binding to the surface or a molecule thereon.

11. The method of claim 1, wherein the set of capture compounds includes at least ten different capture compounds.

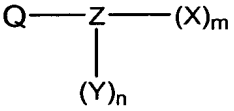
12. The method of claim 1, wherein the set of capture compounds includes at least fifty different capture compounds.

13. The method of claim 1, wherein the set of capture compounds includes at least 100 different capture compounds.

14. The method of claim 1, wherein Q is chemical group for arraying at addressable loci on solid supports.

15. The method of claim 1, wherein:

component capture compounds are selected from the group consisting of compounds that have the formula(e):



$Q\text{-}Z\text{-}(X)_m$ and $Q\text{-}Z\text{-}(Y)_n$;

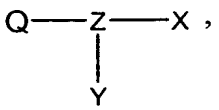
Z is a moiety that is cleavable prior to or during mass spectrometric analysis biomolecules bound to the capture compound;

m is an integer that is 1 to 100; and

n in an integer from 1 to 100.

16. The method of claim 15, wherein:

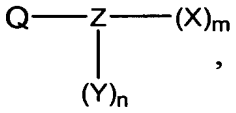
component capture compounds are selected from the group consisting of compounds that have the formula(e):



QZX and Q-Z-Y.

17. The method of claim 1, wherein:

the capture compounds are selected from the group consisting of compounds that have the formula(e):



$Q\text{-}Z\text{-}(X)_m$ and $Q\text{-}Z\text{-}(Y)_n$;

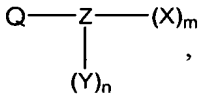
Z is a moiety that is not cleavable prior to or during mass spectrometric analysis of biomolecules bound to the capture compound;

m is an integer that is 1 to 100; and

n in an integer from 1 to 100.

18. The method of claim 17, wherein:

component capture compounds are selected from the group consisting of compounds that have the formula(e):



$Q\text{-}Z\text{-}(X)_m$ and $Q\text{-}Z\text{-}(Y)_n$;

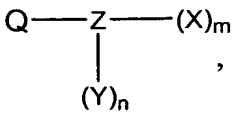
m is an integer that is 1 to 100;

n in an integer from 1 to 100; and

Q is a oligonucleotide or oligonucleotide analog that includes a single-stranded portion of sufficient length "j" to form a stable hybrid with a base-complementary single stranded nucleic acid molecule or analog.

19. The method of claim 1, wherein:

component capture compounds are selected from the group consisting of

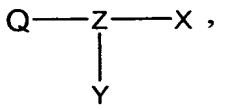


m is an integer that is 1 to 100; and

n is an integer from 1 to 100.

20. The method of claim 3, wherein:

component capture compounds are selected from the group consisting of compounds that the formula(e):



QZX and Q-Z-Y; and

Q is a oligonucleotide or oligonucleotide analog that includes a single-stranded portion of sufficient length "j" to form a stable hybrid with a base-complementary single stranded nucleic acid molecule or analog.

21. The method of claim 3, wherein:

Q is a oligonucleotide or oligonucleotide analog that includes a single-stranded portion of sufficient length to form a stable hybrid with a base-complementary single stranded nucleic acid molecule or analog.

22. The method of claim 3, wherein Q has formula $N^1_sB_iN^2_u$, wherein:

N^1, B and N^2 are oligonucleotides or oligonucleotide analogs comprising s, t and u members, respectively;

B is a region of sequence permutations that contains at least two bases; and

sum of s, i and u is at least 5.

23. The method of claim 22, wherein the sum of s, i and u is about 5 up to about 50.

24. The method of claim 22, wherein each member of N^1, B and N^2 is independently selected from among monomer building blocks of deoxyribonucleic acid, ribonucleic acid, protein nucleic acid and analogs thereof.

25. The method of claim 1, wherein Z is a photocleavable, acid cleavable, alkaline cleavable, oxidatively cleavable, or reductively cleavable group.

26. The method of claim 1, wherein Z comprises an insoluble support to which each X, Y and Q is linked either directly or via a linker.

27. The method of claim 26, wherein the insoluble support is selected from the group consisting of a bead, capillary, plate, membrane, wafer, comb, pin, a wafer with pits, an array of pits or nanoliter wells and a flat surface for receiving or linking samples at discrete loci.

28. The method claim 26, wherein the support comprises silicon, silica gel, glass, nylon, Wang resin, Merrifield resin, dextran cross—linked with epichlorohydrin, agarose, cellulose, magnetic beads, Dynabeads, a metal surface or a plastic material.

29. The method of claim 26, wherein Z comprises hydrophobic beads comprising polystyrene, polyethylene, polypropylene or teflon, or hydrophilic beads comprising cellulose, dextran cross—linked with epichlorohydrin, agarose, polyacrylamide, silica gel and controlled pore glass.

30. The method of claim 26, wherein the Z moiety comprises spacer groups S^1 and/or S^2, and a cleavable linkage, where the S^1 and/or S^2 moieties are attached to insoluble support and the cleavable linkage is attached to S^2, if present, otherwise to the insoluble support.

31. The method of claim 1, wherein Z is at least a trivalent moiety selected from straight or branched chain alkylene, straight or branched chain alkenylene, straight or branched chain alkynylene, straight or branched chain alkylenoxy, straight or branched chain alkylenthio, straight or branched chain alkylencarbonyl, straight or branched chain alkylenamino, cycloalkylene, cycloalkenylene, cycloalkynylene, cycloalkylenoxy, cycloalkylenthio, cycloalkylencarbonyl, cycloalkylenamino, heterocyclylene, arylene, arylenoxy, arylenthio, arylencarbonyl, arylenamino, heteroarylene, heteroarylenoxy, heteroarylenthio, heteroarylencarbonyl, heteroarylenamino, oxy, thio, carbonyl, carbonyloxy, ester, amino, amido, phosphino, phosphineoxido,

phosphoramidato, phosphinamidato, sulfonamido, sulfonyl, sulfoxido, carbamato, ureido, and combinations thereof, and is unsubstituted or substituted with one or more substituents each independently selected from R^{15};

each R^{15} is independently a monovalent group selected from straight or branched chain alkyl, straight or branched chain alkenyl, straight or branched chain alkynyl, cycloalkyl, cycloalkenyl, cycloalkynyl, heterocyclyl, straight or branched chain heterocyclylalkyl, straight or branched chain heterocyclylalkenyl, straight or branched chain heterocyclylalkynyl, aryl, straight or branched chain arylalkyl, straight or branched chain arylalkenyl, straight or branched chain arylalkynyl, heteroaryl, straight or branched chain heteroarylalkyl, straight or branched chain heteroarylalkenyl, straight or branched chain heteroarylalkynyl, halo, straight or branched chain haloalkyl, pseudohalo, azido, cyano, nitro, OR^{60}, $NR^{60}R^{61}$, $COOR^{60}$, $C(O)R^{60}$, $C(O)NR^{60}R^{61}$, $S(O)_qR^{60}$, $S(O)_qOR^{60}$, $S(O)_qNR^{60}R^{61}$, $NR^{60}C(O)R^{61}$, $NR^{60}C(O)NR^{60}R^{61}$, $NR^{60}S(O)_qR^{60}$, $SiR^{60}R^{61}R^{62}$, $P(R^{60})_2$, $P(O)(R^{60})_2$, $P(OR^{60})_2$, $P(O)(OR^{60})_2$, $P(O)(OR^{60})(R^{61})$ and $P(O)NR^{60}R^{61}$;

q is an integer from 0 to 2;

each R^{60}, R^{61} and R^{62} is independently hydrogen, straight or branched chain alkyl, straight or branched chain alkenyl, straight or branched chain alkynyl, aryl, straight or branched chain aralkyl, straight or branched chain aralkenyl, straight or branched chain aralkynyl, heteroaryl, straight or branched chain heteroaralkyl, straight or branched chain heteroaralkenyl, straight or branched chain heteroaralkynyl, heterocyclyl, straight or branched chain heterocyclylalkyl, straight or branched chain heterocyclylalkenyl or straight or branched chain heteorcyclylalkynyl;

with the proviso that Z is cleavable prior to or during analysis of the biomolecule.

32. The method of claim 1, wherein Z is at least a trivalent moiety and is selected from straight or branched chain alkyl, straight or branched chain alkenyl, straight or branched chain alkynyl, $(C(R^{15})_2)_d$, O, S, $(CH_2)_d$,

$(CH_2)_dO$, $(CH_2)_dS$, $>N(R^{15})$, $(S(O)_u)$, $(S(O)_2)_w$, $>C(O)$, $(C(O))_w$, $(C(S(O)_u))_w$, $(C(O)O)_w$, $(C(R^{15})_2)_dO$, $(C(R^{15})_2)_dS(O)_u$, $O(C(R^{15})_2)_d$, $S(O)_u(C(R^{15})_2)_d$, $(C(R^{15})_2)_dO(C(R^{15})_2)_d$, $(C(R^{15})_2)_dS(O)_u(C(R^{15})_2)_d$, $N(R^{15})(C(R^{15})_2)_d$, $(C(R^{15})_2)_dNR^{15}$, $(C(R^{15})_2)_dN(R^{15})(C(R^{15})_2)_d$, $-(CH_2)_dC(O)N(CH_2)_d-$, $-(CH_2)_dC(O)N(CH_2)_dC(O)N(CH_2)_d-$, $(S(R^{15})(O_u)_w$, $(C(R^{15})_2)_d$, $(C(R^{15})_2)_dO(C(R^{15})_2)_d$, $(C(R^{15})_2)_d(C(O)O)_w(C(R^{15})_2)_d$, $(C(O)O)_w(C(R^{15})_2)_d$, $(C(R^{15})_2)_d(C(O)O)_w$, $(C(S)(R^{15})_w$, $(C(O))_w(CR^{15}{}_2)_d$, $(CR^{15})_d(C(O))_w(CR^{15})_d$, $(C(R^{15})_2)_d(C(O))_w$, $N(R^{15})(C(R^{15})_2)_w$, $OC(R^{15})_2C(O)$, $O((R^{15})_2C(O)N(R^{15})$, $(C(R^{15})_2)_wN(R^{15})(C(R^{15})_2)_w$, $(C(R^{15})_2)_wN(R^{15})$, $>P(O)_v(R^{15})_x$, $>P(O)_u(R^{15})_3$, $>P(O)_u(C(R^{15})_2)_d$, $>Si(R^{15})_2$ and combinations of any of these groups;

u, v and x are each independently 0 to 5;

each d is independently an integer from 1 to 20, or 1 to 12, or 1-6, or 1 to 3;

each w is independently an integer selected from 1 to 6, or 1 to 3, or 1 to 2;

with the proviso that Z is cleavable prior to or during analysis of the biomolecule.

33. The method of claim 1, wherein Z is a trivalent moiety having any combination selected from the group consisting of arylene, heteroarylene, cycloalkylene, $>C(R^{15})_2$, $C(R^{15})=C(R^{15})$, $>C=C(R^{23})(R^{24})$, $>C(R^{23})(R^{24})$, $C\equiv C$, O, $>S(A)_u$, $>P(D)_v(R^{15})$, $>P(D)_v(ER^{15})$, $>Si(R^{15})_2$, $>N(R^{15})$, $>N^+(R^{23})(R^{24})$ and $>C(E)$; where u is 0, 1 or 2; v is 0, 1, 2 or 3; A is O or NR^{15}; D is S or O; and E is S, O or NR^{15}; that groups can be combined in any order;

each R^{15} is a monovalent group independently selected from the group consisting of hydrogen and Y^1R^{18};

each Y^1 is a divalent group independently having any combination of the following groups: a direct link, arylene, heteroarylene, cycloalkylene, $>C(R^{17})_2$, $C(R^{17})=C(R^{17})$, $>C=C(R^{23})(R^{24})$, $>C(R^{23})(R^{24})$, $C\equiv C$, O, $>S(A)_u$, $>P(D)_v(R^{17})$, $>P(D)_v(ER^{17})$, $>N(R^{17})$, $>N(COR^{17})$, $>N^+(R^{23})(R^{24})$, $>Si(R^{17})_2$ and $>C(E)$; where u is 0, 1 or 2; v is 0, 1, 2 or 3; A is O or NR^{17}; D is S or O; and E is S, O or NR^{17}; that groups can be combined in any order;

R^{17} and R^{18} are each independently selected from the group consisting of hydrogen, halo, pseudohalo, cyano, azido, nitro, $SiR^{27}R^{28}R^{25}$, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and $NR^{19}R^{20}$;

R^{19} and R^{20} are each independently selected from hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl and heterocyclyl;

R^{23} and R^{24} are selected from (i) or (ii) as follows:

(i) R^{23} and R^{24} are independently selected from the group consisting of hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl and heteroaryl; or

(ii) R^{23} and R^{24} together form alkylene, alkenylene or cycloalkylene;

R^{25}, R^{27} and R^{28} are each independently a monovalent group selected from hydrogen, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and $NR^{19}R^{20}$;

R^{15}, R^{17}, R^{18}, R^{19}, R^{20}, R^{23}, R^{24}, R^{25}, R^{27} and R^{28} can be substituted with one or more substituents each independently selected from Z^2; Z^2 is selected from alkyl, alkenyl, alkynyl, aryl, cycloalkyl, cycloalkenyl, hydroxy, $S(O)_hR^{35}$; h is 0, 1 or 2, $NR^{35}R^{36}$, $COOR^{35}$, COR^{35}, $CONR^{35}R^{36}$, $OC(O)NR^{35}R^{36}$, $N(R^{35})C(O)R^{36}$, alkoxy, aryloxy, heteroaryl, heterocyclyl, heteroaryloxy, heterocyclyloxy, aralkyl, aralkenyl, aralkynyl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, aralkoxy, heteroaralkoxy, alkoxycarbonyl, carbamoyl, thiocarbamoyl, alkoxycarbonyl, carboxyaryl, halo, pseudohalo, haloalkyl and carboxamido;

R^{35} and R^{36} are each independently selected from among hydrogen, halo, pseudohalo, cyano, azido, nitro, trialkylsilyl, dialkylarylsilyl, alkyldiarylsilyl, triarylsilyl, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl,

aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy, amino, amido, alkylamino, dialkylamino, alkylarylamino, diarylamino and arylamino;

with the proviso that Z is cleavable prior to or during analysis, including mass spectrometric analysis of the compound.

34. The method of claim 1, wherein Z has the formula: $(S^1)_tM(R^{15})_a(S^2)_bL$, wherein:

S^1 and S^2 are spacer moieties;

t and b are each independently 0 or 1;

a is an integer from 0 to 4;

M is a central moiety possessing three or more points of attachment;

each R^{15} is a monovalent group independently selected from Y^2R^{18};

each Y^2 is a divalent group independently having any combination of the following groups: a direct link, arylene, heteroarylene, cycloalkylene, $>C(R^{17})_2$, $C(R^{17})=C(R^{17})$, $>C=C(R^{23})(R^{24})$, $>C(R^{23})(R^{24})$, $C\equiv C$, O, $>S(A)_u$, $>P(D)_v(R^{17})$, $>P(D)_v(ER^{17})$, $>N(R^{17})$, $>N(COR^{17})$, $>N^+(R^{23})(R^{24})$, $>Si(R^{17})_2$ and >C(E); where u is 0, 1 or 2; v is 0, 1, 2 or 3; A is O or NR^{17}; D is S or O; and E is S, O or NR^{17}; that groups can be combined in any order;

R^{17} and R^{18} are each independently selected from the group consisting of hydrogen, halo, pseudohalo, cyano, azido, nitro, $SiR^{27}R^{28}R^{25}$, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and $NR^{19}R^{20}$;

R^{19} and R^{20} are each independently selected from hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl and heterocyclyl;

R^{23} and R^{24} are selected from (i) or (ii) as follows:

(i) R^{23} and R^{24} are independently selected from the group consisting of

hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl and heteroaryl; or

(ii) R^{23} and R^{24} together form alkylene, alkenylene or cycloalkylene;

R^{25}, R^{27} and R^{28} are each independently a monovalent group selected from hydrogen, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and $NR^{19}R^{20}$;

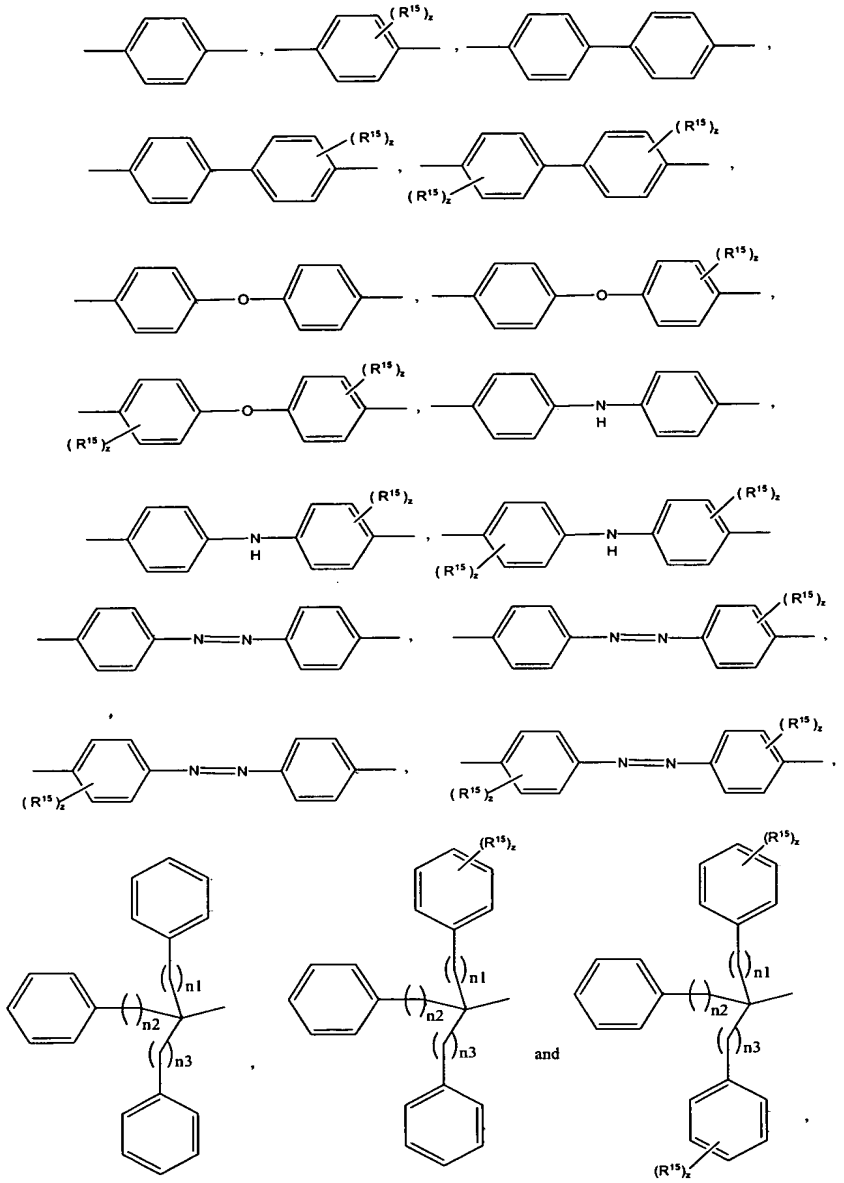
R^{15}, R^{17}, R^{18}, R^{19}, R^{20}, R^{23}, R^{24}, R^{25}, R^{27} and R^{28} can be substituted with one or more substituents each independently selected from Z^2; Z^2 is selected from alkyl, alkenyl, alkynyl, aryl, cycloalkyl, cycloalkenyl, hydroxy, $S(O)_hR^{35}$; h is 0, 1 or 2, $NR^{35}R^{36}$, $COOR^{35}$, COR^{35}, $CONR^{35}R^{36}$, $OC(O)NR^{35}R^{36}$, $N(R^{35})C(O)R^{36}$, alkoxy, aryloxy, heteroaryl, heterocyclyl, heteroaryloxy, heterocyclyloxy, aralkyl, aralkenyl, aralkynyl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, aralkoxy, heteroaralkoxy, alkoxycarbonyl, carbamoyl, thiocarbamoyl, alkoxycarbonyl, carboxyaryl, halo, pseudohalo, haloalkyl and carboxamido;

R^{35} and R^{36} are each independently selected from among hydrogen, halo, pseudohalo, cyano, azido, nitro, trialkylsilyl, dialkylarylsilyl, alkyldiarylsilyl, triarylsilyl, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy, amino, amido, alkylamino, dialkylamino, alkylarylamino, diarylamino and arylamino; and

L is a group that is cleavable prior to or during mass spectrometric analysis of the compound.

35. The method of claim 34, wherein M is a tetravalent alkylene, tetravalent phenylene, tetravalent biphenylene or a tetravalent heterobifunctional trityl derivative, and is unsubstituted or is substituted with 1 to 4 groups, each independently selected from R^{15}.

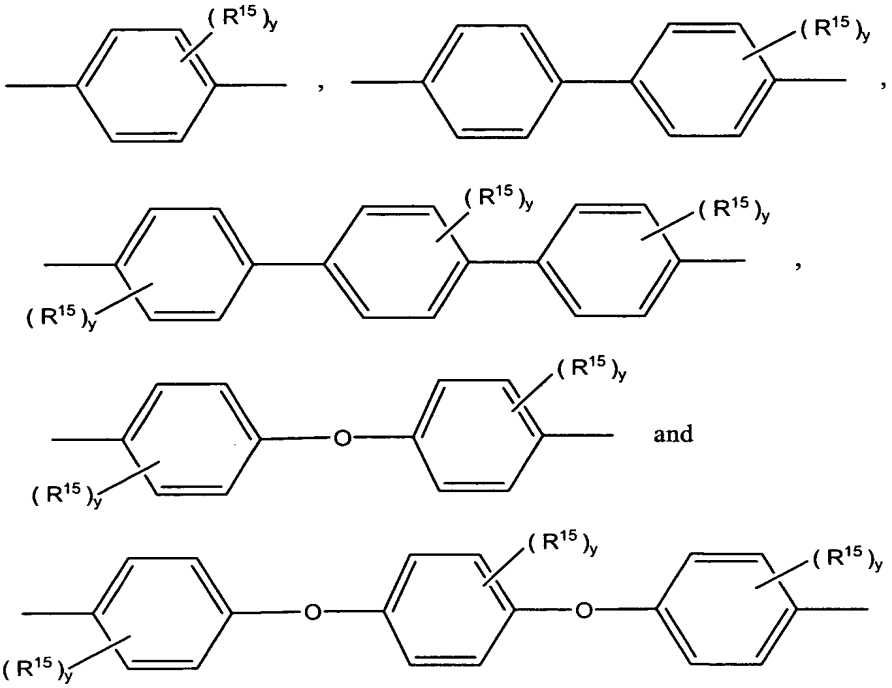
36. The method of claim 34, wherein M is at least a trivalent group selected from the following groups absent a hydrogen atom: $(CH_2)_r$, $(CH_2O)_r$, $(CH_2CH_2O)_r$, $(NH(CH_2)_rC(=0))_s$, $(NHCH(R^{52})C(=O))_r$, $(O(CH)_rC(=0))_s$,



wherein r and s are each independently an integer from 1 to 10; R^{52} is the side chain of a natural or unnatural α-amino acid; z is an integer from 1 to 4 and n1, n2 and n3 are each independently an integer from 0 to 4.

37. The method of claim 34, wherein S^1 and S^2 are each independently selected from $(CH_2)_r$, (CH_2O), $(CH_2CH_2O)_r$,$(NH(CH_2)_rC(=O))_s$,

$(NHCH(R^{52})C(=O))_s$, $(O(CH)_rC(=0))_s$,



and

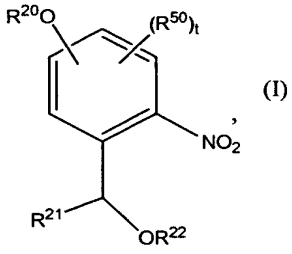
wherein r and s are each independently an integer from 1 to 10; R^{52} is the side chain of a natural or unnatural α-amino acid; and y is an integer from 0 to 4.

38. The method of claim 34, wherein L is a disulfide moiety, a photocleavable group, an acid cleavable group, an alkaline cleavable group, a oxidatively cleavable group, or a reductively cleavable group.

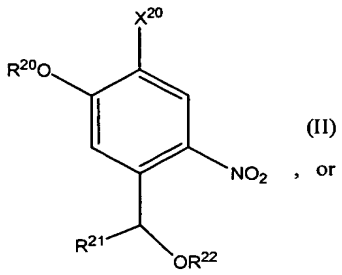
39. The method of claim 34, wherein L is a trityl ether, an ortho nitro substituted aryl group, an o-nitrobenzyl, a phenacyl, nitrophenylsulfenyl group.

40. The method of claim 34, wherein:

L has formula I, II or III as follow:

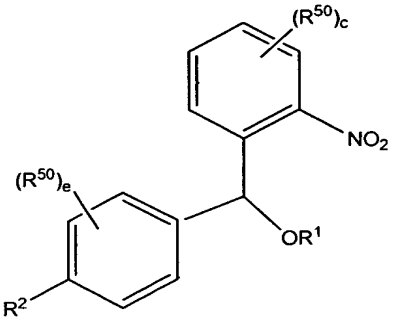


(I)



(II)

, or



(III)

R^{20} is ω(4,4'dimethoxytrityloxy)alkyl or ωhydroxyalkyl; R^{21} is selected from hydrogen, alkyl, aryl, alkoxycarbonyl, aryloxycarbonyl and carboxy;

R^{21} is selected from hydrogen, alkyl, aryl, alkoxycarbonyl, aryloxycarbonyl and carboxy;

R^{22} is hydrogen; t is 0-3;

R^{50} is alkyl, alkoxy, aryl or aryloxy;

X^{20} is hydrogen, alkyl or OR^{20}..

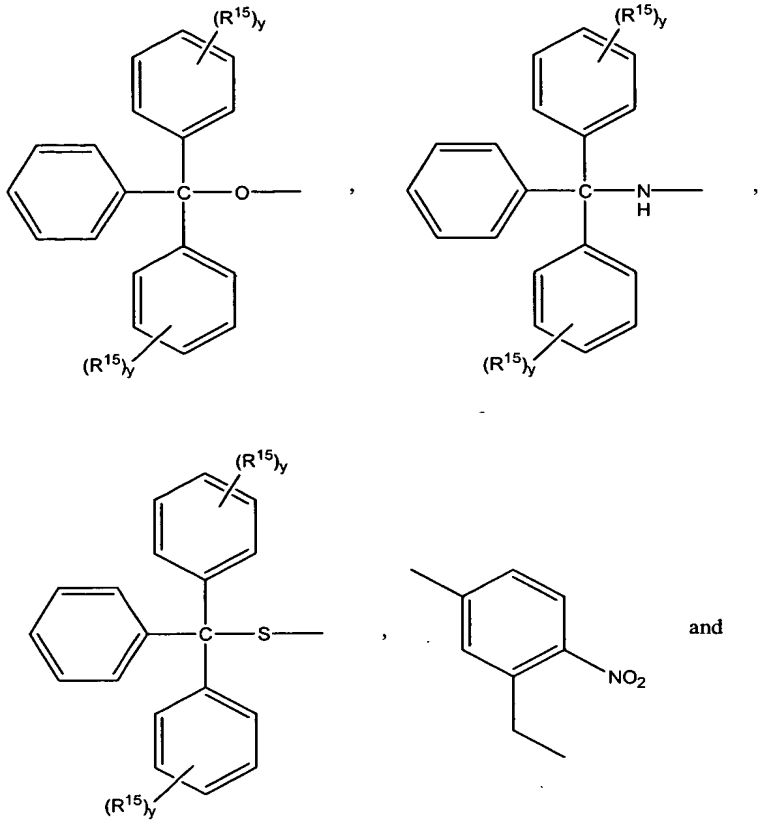
R^1 is hydrogen;

R^2 is selected from among ω-hydroxyalkoxy, ω-(4,4'-dimethoxytrityloxy)alkoxy, ω-hydroxyalkyl and ω-(4,4'-dimethoxytrityloxy)alkyl, and is unsubstituted or substituted on the alkyl or alkoxy chain with one or more alkyl groups; and

c and e are each independently 0-4.

41. The method of claim 34, wherein:

L is selected from among SS, $OP(=O)(OR^{51})NH$, $pMeONO_2PhCH_2$, OC(=O), and



R^{51} is straight or branched chain alkyl, straight or branched chain alkenyl, straight or branched chain alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, straight or branched chain aralkyl, straight or branched chain aralkenyl, straight or branched chain aralkynyl, straight or branched chain heteroaralkyl, straight or branched chain heteroaralkenyl, straight or branched chain heteroaralkynyl, straight or branched chain cycloalkylalkyl, straight or branched chain cycloalkylalkenyl, straight or branched chain cycloalkylalkynyl, straight or branched chain heterocyclylalkyl, straight or branched chain heterocyclylalkenyl or straight or branched chain heterocyclylalkynyl; and

y is an integer from 0 to 4.

42. The method of claim 34, wherein R^{15} is H, OH, OR^{51}, SH, SR^{51}, NH_2, NHR^{51}, $N(R^{51})_2$, F, Cl, Br, I, SO_3H, PO^2_4, CH_3, CH_2CH_3, $CH(CH_3)_2$ or $C(CH_3)_3$; where R^{51} is straight or branched chain alkyl, straight or branched chain alkenyl, straight or branched chain alkynyl, aryl, heteroaryl, cycloalkyl,

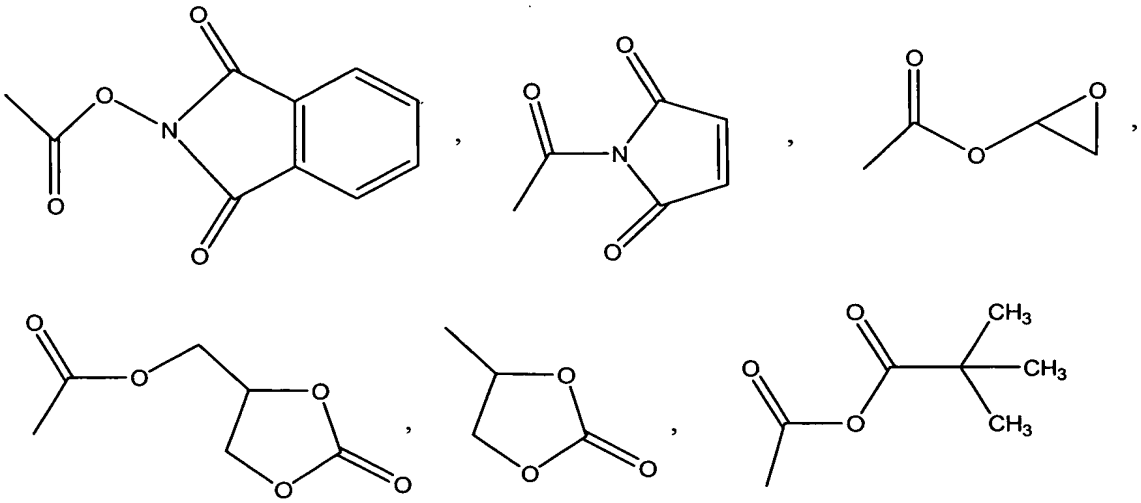
heterocyclyl, straight or branched chain aralkyl, straight or branched chain aralkenyl, straight or branched chain aralkynyl, straight or branched chain heteroaralkyl, straight or branched chain heteroaralkenyl, straight or branched chain heteroaralkynyl, straight or branched chain cycloalkylalkyl, straight or branched chain cycloalkylalkenyl, straight or branched chain cycloalkylalkynyl, straight or branched chain heterocyclylalkyl, straight or branched chain heterocyclylalkenyl or straight or branched chain heterocyclylalkynyl.

43. The method of claim 1, wherein each X is selected from the group consisting of an active ester, an active halo moiety, an amino acid side chain-specific functional group, a reagent that binds to active site of an enzyme, a ligand that binds to a receptor, a specific peptide that binds to a biomolecule surfaces, a lectin, an antibody, an antigen, biotin; streptavidin.

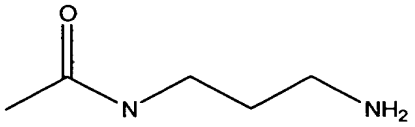
44. The method of claim 1, wherein an X is an α-halo ether, an α-halo carbonyl group, maleimido, a metal complex, an expoxide, an isothiocyanate, or an antibody against phosphorylated or glycosylated peptides/proteins.

45. The method of claim 1, wherein X is $C(=O)OPhpNO_2$, $C(=O)OC_6F_5$, C(=O)O(Nsuccinimidyl), OCH_2I, OCH_2Br, OCH_2Cl, $C(O)CH_2I$, $C(O)CH_2Br$ or $C(O)CH_2Cl$.

46. The method of claim 1, wherein X is



or



47. The method of claim 1, wherein member compounds comprise a mass modifying tag linked to Z.

48. The method of claim 30, wherein member compounds comprise a mass modifying tag; and the mass modifying tag is linked to Z or is S^2.

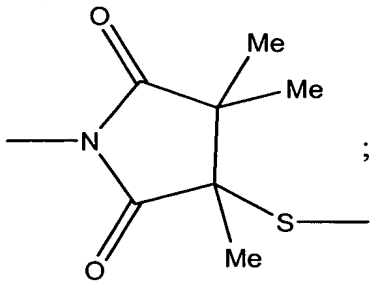
49. The method of claim 34, wherein:

the mass modified Z moiety has the formula: $(S^1)_tM(R^{15})_a(S^2)_bLT$; and

T is a mass modifying tag.

50. The method of calim 47, wherein the mass modifying tag is a divalent group having the formula X^1R^{10} and is selected from (i)-(vii) as follows:

(i) X^1 is a divalent group selected from O, $OC(O)(CH_2)_yC(O)O$, NHC(O), C(O)NH, $NHC(O)(CH_2)_yC(O)O$, NHC(S)NH, OP(O-alkyl)O, OSO_2O, $OC(O)CH_2S$, S, NH and



; and

R^{10} is a divalent group selected from $(CH_2CH_2O)_zCH_2CH_2O$, $(CH_2CH_2O)_zCH_2CH_2O$alkylene, alkylene, alkenylene, alkynylene, arylene, heteroarylene, $(CH_2)_zCH_2O$, $(CH_2)_zCH_2O$alkylene, $(CH_2CH_2NH)_zCH_2CH_2NH$, $CH_2CH(OH)CH_2O$, $Si(R^{12})(R^{13})$, CHF and CF_2; where y is an integer from 1 to 20; z is an integer from 0 to 200; R^{11} is the side chain of a naturally occurring á-amino acid; and R^{12} and R^{12} are each independently selected from alkyl, aryl and aralkyl;

(ii) SS;

(iii) S;

(iv) $(NH(CH_2)_yNHC(O)(CH_2)_yC(O))_zNH(CH_2)_yNHC(O)$-$(CH_2)_yC(O)O$, where y and z are selected as in (i);

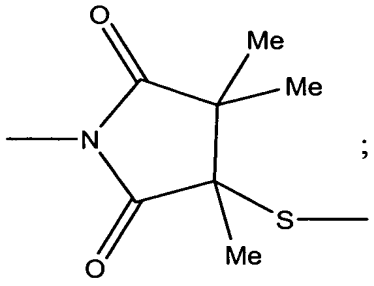
(v) $(NH(CH_2)_yC(O))_zNH(CH_2)_yC(O)O$, where y and z are selected as in (i);

(vi) $(NHCH(R^{11})C(O))_zNHCH(R^{11})C(O)O$, where R^{11} and z are selected as in (i); or

(vii) $(O(CH_2)_yC(O))_zNH(CH_2)_yC(O)O$, where y and z are selected as in (i).

51. The method of claim 48, wherein S^2 has the formula X^1R^{10}, where X^1R^{10} is selected from (i)-(vii) as follows:

(i) X^1 is a divalent group selected from O, $OC(O)(CH_2)_yC(O)O$, NHC(O), C(O)NH, $NHC(O)(CH_2)_yC(O)O$, NHC(S)NH, OP(O-alkyl)O, OSO_2O, $OC(O)CH_2S$, S, NH and



; and

R^{10} is a divalent group selected from $(CH_2CH_2O)_zCH_2CH_2O$, $(CH_2CH_2O)_zCH_2CH_2O$alkylene, alkylene, alkenylene, alkynylene, arylene, heteroarylene, $(CH_2)_zCH_2O$, $(CH_2)_zCH_2O$alkylene, $(CH_2CH_2NH)_zCH_2CH_2NH$, $CH_2CH(OH)CH_2O$, $Si(R^{12})(R^{13})$, CHF and CF_2; where y is an integer from 1 to 20; z is an integer from 0 to 200; R^{11} is the side chain of a naturally occurring α-amino acid; and R^{12} and R^{12} are each independently selected from alkyl, aryl and aralkyl;

(ii) SS;

(iii) S;

(iv) $(NH(CH_2)_yNHC(O)(CH_2)_yC(O))_zNH(CH_2)_yNHC(O)$-$(CH_2)_yC(O)O$, where y and z are selected as in (i);

(v) $(NH(CH_2)_yC(O))_zNH(CH_2)_yC(O)O$, where y and z are selected as in (i);

(vi) $(NHCH(R^{11})C(O))_zNHCH(R^{11})C(O)O$, where R^{11} and z are selected as in (i); or

(vii) $(O(CH_2)_yC(O))_zNH(CH_2)_yC(O)O$, where y and z are selected as in (i).

52. The method of claim 3, wherein Q is an oligonucleotide comprising at least "j" nucleotides; and the collection comprises about 10 to 4^j compounds of any, wherein, where j is the number of bases in the single-stranded portion of the oligonucleotide.

53. The method of claim 52, wherein Z is a moiety that is cleavable during mass spectrometric analysis of the compounds.

54. The method of claim 52, wherein Z is a moiety that is not cleavable during mass spectrometric analysis of the compounds.

55. The method of claim 3, wherein a composition, comprising the collection of capture compounds is hybridized to a plurality of oligonucleotides or analogs thereof that comprise oligonucleotides that are complementary to each each Q.

56. The method of claim 55, wherein the oligonucleotides or analog thereof that are complementary to Q are immobilized on a solid support as an array.

57. The method of claim 56, wherein the support is an addressable array.

58. The method of claim 1, wherein the biomolecules are covalently bound to the capture compounds.

59. The method of claim 58, wherein the biomolecules comprise proteins.

60. The method of claim 58, wherein the biomolecules comprise receptors.

61. The method of claim 58, wherein the biomolecules comprise enzymes.

62. The method of claim 1, wherein capture compounds comprise:

a central core Z linked to a reactive functionality X and a selectivity functionality Y, whereby a capture compound forms a covalent bond with a biomolecule in the mixture or interacts with high stability such that the affinity of binding of the capture compound to the biomolecule through the reactive functionality in the presence of the selectivity functionality is at least ten-fold greater than in the absence of the selectivity functionality.

63. The method of claim 3, wherein compounds in the collection comprises Z, which comprises a reagent of a luminescence assay or a group that is detected in a colorimetric assay; and a sorting group Q that comprises a single-stranded oligonucleotide.

64. The method of claim 19, wherein Z is a solid support.

65. The method of claim 19, wherein Z is a particulate support.

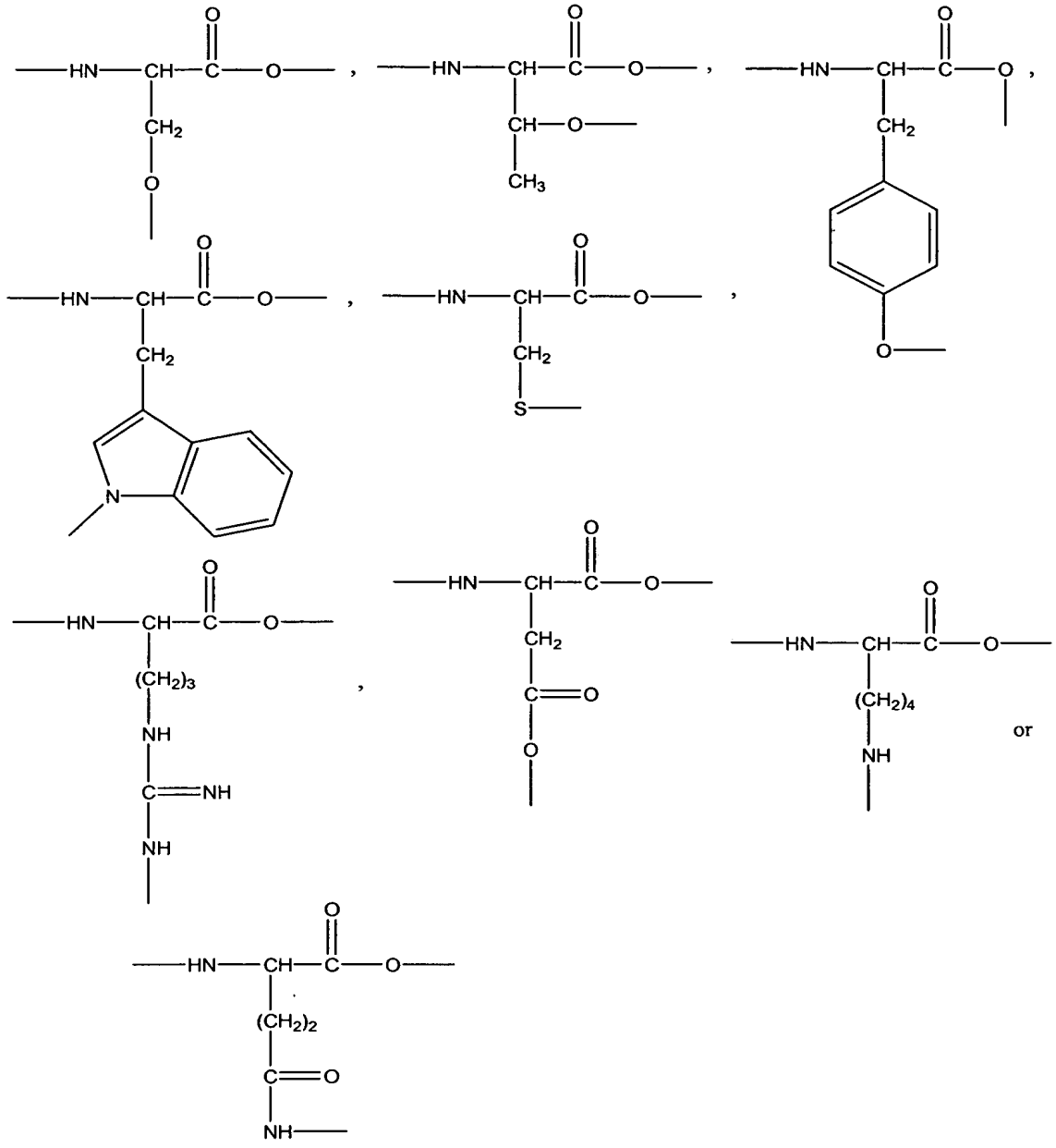
66. The method of claim 1, wherein the capture compounds further comprise a solubility group W that influences the solubility properties of the capture compound.

67. The method of claim 1, wherein the selectivity function Y is selected from those set forth in Figure 17 and/or the reactivity function X is selected from those set forth in Figure 16.

68. The method of claim 1, wherein the selectivity function Y is selected from those set forth in Figure 21 and/or the reactivity function X is selected from those set forth in Figure 16.

69. The method of claim 1, wherein the selectivity function Y is a pharmaceutical drug selected from atorvastatin, celecoxib, refecoxib and cerivastatin.

70. The method of claim 36, wherein M is



71. The method of claim 36, wherein n3 is 2.

72. The method of claim 1, wherein the X moiety is linked to the Z moiety via a spacer.

73. The method of claim 72, wherein the spacer is $(CH_2)_r$, (CH_2O), $(CH_2CH_2O)_r$,$(NH(CH_2)_rC(=O))_s$, $(O(CH)_rC(=O))_s$, $-((CH_2)_{r1}-C(O)NH-(CH_2)_{r2})_s-$ or-$(C(O)NH-(CH_2)_r)_s-$., where r, r1, r2 and s are each independently and integer from 1 to 10.

74. The method of claim 3 wherein Q is biotin, hexa-His, 4,4-difluoro-4-bora-3a,4a-diaza-*s*-indacene, oligonucleotides, nucleosides, nucleotides, antibodies, immunotoxin conjugates, adhesive peptides, lectins, liposomes, protein nucleic acids, activated dextrans or peptides.

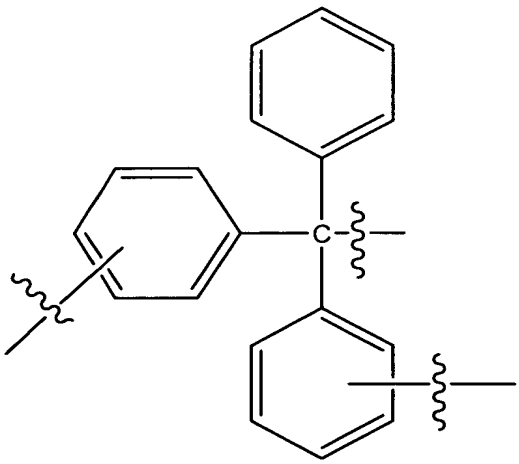
75. The method of claim 3 wherein Q is biotin.

76. A method of identifying drug non-target biomolecules in a mixture of biomolecules, comprising:

interacting mixture of biomolecules with a capture compound, wherein the capture compound comprises a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomlecules when the selectivity moiety is present than in its absence; a moiety Q, wherein Q permits sorting; and a moiety Z for presenting X, Y and Q; and

analyzing the captured biomolecules to identify drug non-target.

77. The method of claim 76, wherein Z has the formula:



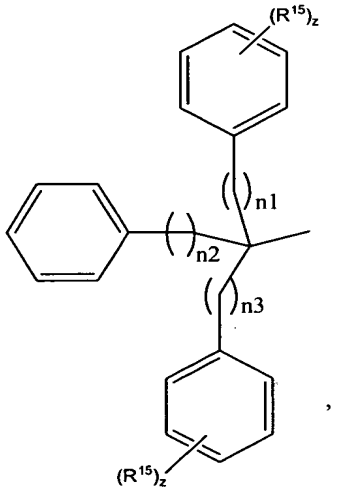
78. The method of claim 76, wherein X is selected from the groups set forth in Figure 16.

79. The method of claim 76, wherein Y is selected from the groups

set forth in Figure 17.

80. The method of claim 76, wherein Q is an oligonucleotide or oligonucleotide analog that includes a single-stranded portion of sufficient length "j" to form a stable hybrid with a base-complementary single stranded nucleic acid molecule or analog.

81. A collection of capture compounds, comprising a plurality of capture compounds, comprising sets of capture compounds, wherein each set of capture compounds includes a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomlecules when the selectivity moiety is present than in its absence; and a moiety Z for presenting X and Y, wherein the moiety Z is



wherein R^{15} as described above, n1, n2, n3 are 0 to 4 with the proviso that all n1, n2 and n3 are not equal to 0 at the same time.

82. A capture compound selected from figure 23.

83. A method for analysis of biomolecules, comprising:

a) contacting a composition comprising a biomolecule with a capture compound or a collection of capture compounds of claim 81 to form capture compound-biomolecule complexes; and

b) identifying or detecting bound biomolecules.

84. The method of claim 83, wherein the biomolecules are proteins.

85. The method of claim 83, wherein the capture compounds include a biotin moiety.

86. The method of claim 83, wherein:

the capture compounds are in an addressable array; and

each locus in the array contains a different set of capture compounds.

87. The method of claim 83, wherein identification comprises mass spectrometric analysis of the bound biomolecules.

88. The method of claim 83, wherein the biomolecules are proteins.

89. The method of claim 88, wherein the biomolecules are receptors.

90. The method of claim 88, wherein the biomolecules are enzymes.

91. The method of claim 87, wherein the biomolecules bound to the capture compounds are treated with a protease prior to mass spectrometric analysis.

92. The method of claim 87, wherein each set of compounds in the collection comprises the same reactivity function but differs in selectivity function.

93. The method of claim 87, wherein each set of compounds in the collection comprises different reactivity function, selectivity function and sorting function.

94. The method of claim 87, wherein each set of compounds in the collection comprises different reactivity function and selectivity function.

95. A method for separating protein conformers, comprising:

contacting a composition comprising a biomolecule with a collection of capture compounds of claim 81,

separating the members of the collection; and

identifying the bound proteins from the mixture, whereby each conformer has different binding specificity for members of the collection.

96. The method of claim 95, wherein identification is effected by mass spectrometry.

97. The method of claim 95, wherein at least one conformer is associated with a disease.

98. A method for reducing diversity of complex mixture of biomolecules, comprising:

contacting the mixture with a collection of capture compounds of claim 81 to form complexes of capture compounds with bound biomolecules; and either before, during or after contacting,

separating each set of complexes of capture compounds with biomolecules from the other sets.

99. A method for identification of phenotype-specific biomolecules, comprising:

sorting cells from a single subject according to a predetermined phenotype to produce at least two separated sets of cells;

contacting mixtures of biomolecules from each set of sorted cells with a collection of capture compounds of claim 81; and

comparing the patterns of biomolecules binding from each set to identify biomolecules that differ for each set, thereby identifying phenotype-specific biomolecules.

100. The method of claim 99, wherein the cells are synchronized or frozen in a metabolic state before sorting and/or after sorting.

101. The method of claim 99, wherein the biomolecules comprise proteins.

102. The method of claim 99, wherein the bound biomolecules are identified by mass spectrometry.

103. The method of claim 99, wherein each capture compound includes selectivity function that covalently binds to proteins; a moiety that increases the selectivity of the binding such that the capture compound binds to fewer proteins when the selectivity moiety is present than in its absence.

104. The method of claim 99, wherein each capture compound

further comprises a sorting function for arraying of the capture compounds at different loci on a solid support.

105. The method of claim 99, wherein capture compounds comprise a reactive function that covalently binds to proteins; and a sorting function that permits arraying of the capture compounds on a solid support by binding to the surface or a molecule thereon.

106. The method of claim 99, wherein the phenotypes are diseased and healthy phenotypes.

107. The method of claim 106, wherein the cells are disease phenotype is a tumor and the healthy phenotype is non-tumor.

108. The method of claim 83, wherein the contacting step is performed in an aqueous medium and the biomolecules are hydrophilic.

109. The method of claim 83, wherein the contacting step is performed in a hydrophobic medium and the biomolecules are hydrophobic.

110. The method of claim 83, wherein identification or detection is effected by mass spectrometric analysis of the biomolecule-capture compound complexes.

111. The method of claim 110, wherein the mass spectrometric format is matrix assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry.

112. The method of claim 83, wherein the biomolecules comprise proteins.

113. The method of claim 110, wherein mass spectrometric analysis of the bound biomolecules, comprises:

(i) addition of matrix to the biomolecule-capture agent complexes;

(vi) spot-by-spot matrix assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry.

114. The method of claim 83, further comprising:

chemical or enzymatic treatment of the biomolecule-capture compound complexes to remove or cleave portions thereof.

115. The method of claim 87, wherein mass spectrometric analysis of the bound biomolecules, comprises:

(i) addition of matrix to the sets of biomolecule-capture agent complexes; and

(ii) matrix assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry of each set of biomolecule-capture agent complexes.

116. The method of claim 83 wherein the composition comprising a biomolecule is a cell lysate.

117. The method of claim 116, wherein the cells from which the lysate is produced are synchronized or frozen in a metabolic state.

118. A system for analysis of mixtures of biomolecules, comprising:

a collection of capture compounds of claim 81;

a computer programmed with instructions for controlling and directing analysis of biomolecules using the collections;

a mass spectrometer; and

software for analysis of data produced by the mass spectrometer.

119. The system of claim 118 that is an automated system.

120. The system of claim 113, further comprising a liquid chromatographic device.

121. A method of processing the mass spectrometric data produced by the method of claim 82, comprising:

(a) subtracting any background;

(b) reducing noise;

(c) calibrating molecular weight; and

(d) refining peaks.

122. The method of claim 122, wherein step (d) comprises peak integration.

123. The method of claim 121, further comprising:

(e) comparing the processed data with existing protein databases

or DNA databases containing open reading frames to determine whether the protein is known, and

(f) if the protein is known, identifying modifications

124. The method of claim 121, further comprising:

comparing data from tissues of healthy and diseased individuals, or from different physiological or developmental stages, or from different parts of a tissue.to form double stranded hybrids and

analyzing the double stranded hybridized complexes.

125. The method of claim 87, wherein the analysis is orthogonal time of flight (O-TOF) mass spectrometry.

126. The method of claim 87, wherein the analysis is electrospray (ES) mass spectrometry.

127. A method for analyzing biomolecule interactions, comprising:

a) contacting a mixture of biomolecules with a collection of capture compounds of claim 81, to form a compound-biomolecule complexes, wherein:

the central core is not cleavable prior to or during mass spectrometric analysis of biomolecules bound to the capture compound; and

the complexes are stable to matrix assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry conditions;

b) contacting the capture compound-biomolecule complexes with a mixture containing compounds selected from the group consisting of mixtures of biomolecules and small molecules test compounds, wherein compounds in the mixture bind to biomolecules in the complexes;

c) before or after step b) immobilizing the capture compounds on a solid support via the sorting group of each set of capture compounds;

d) analyzing the bound compounds by mass spectrometry.

128. The method of claim 127, wherein the small molecule test compounds are candidates drugs and are selected from the group consisting of small organic molecules, peptides, peptide mimetics, antisense molecules

or dsRNA, antibodies, fragments of antibodies and recombinant or synthetic antibodies and fragments thereof; and

the method is a method for identifying candidate drugs that bind to biomolecules.

129. The method of claim 127, wherein the capture compound-biomolecule complexes are contacted in step a) with a mixture of biomolecules to identify components of biomolecule complexes or biochemical pathways.

130. The method of claim 127, wherein the biomolecules are proteins.

131. A method of analysis of biomolecules, comprising:

a) contacting a composition comprising a biomolecule with a collection plurality of capture compounds, comprising sets of capture compounds, wherein each set of capture compounds includes a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomolecules when the selectivity moiety is present than in its absence; a moiety Q, such that each set contains a different Q, wherein Q permits separation of each set and a moiety Z for presenting X , Y and Q;

b) digesting the captured biomolecules by chemical or enzymatic treatment;

c) separating each set of captured compounds based on the sorting moiety Q; and

d) analyzing each set of capture compounds to identify the biomolecules.

132. A method of analysis of biomolecules, comprising:

a) contacting a composition comprising a biomolecule with a collection capture compounds, wherein each capture compound comprises a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently

high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomlecules when the selectivity moiety is present than in its absence; a moiety Q, wherein Q permits sorting; and a moiety Z for presenting X, Y and Q;

b) separating each set of captured compounds based on the sorting moiety Q;

c) digesting the captured biomolecules by chemical or enzymatic treatment; and

d) analyzing each set of capture compounds to identify the biomolecules.

133. The method of claim 83, wherein:

the capture compounds comprise a sorting function for arraying the compounds on a solid support; and

the method further comprises arraying the capture compounds on a solid support before, during or after the contacting step, wherein:

the resulting biomolecule-capture compound complexes are at discrete spots on a solid support.

134. The method of claim 133, wherein mass spectrometric analysis of the bound biomolecules, comprises:

(i) addition of matrix to the biomolecule-capture agent complexes;

(vi) spot-by-spot matrix assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry.

135. A solid support, comprising the collection of compounds of claims 81, wherein each set of compounds is arrayed at a single locus.

136. The solid support of claim 135, wherein the array is an addressable array.

137. The method of claim 1, wherein Z has the formula: $(S^1)_t M(R^{15})_a(S^2)_b$, wherein:

S^1 and S^2 are spacer moieties;

t and b are each independently 0 or 1;

a is an integer from 0 to 4;

M is a central moiety possessing three or more points of attachment;

each R^{15} is a monovalent group independently selected from Y^2R^{18};

each Y^2 is a divalent group independently having any combination of the following groups: a direct link, arylene, heteroarylene, cycloalkylene, $>C(R^{17})_2$, $C(R^{17})=C(R^{17})$, $>C=C(R^{23})(R^{24})$, $>C(R^{23})(R^{24})$, $C\equiv C$, O, $>S(A)_u$, $>P(D)_v(R^{17})$, $>P(D)_v(ER^{17})$, $>N(R^{17})$, $>N(COR^{17})$, $>N^+(R^{23})(R^{24})$, $>Si(R^{17})_2$ and >C(E); where u is 0, 1 or 2; v is 0, 1, 2 or 3; A is O or NR^{17}; D is S or O; and E is S, O or NR^{17}; that groups can be combined in any order;

R^{17} and R^{18} are each independently selected from the group consisting of hydrogen, halo, pseudohalo, cyano, azido, nitro, $SiR^{27}R^{28}R^{25}$, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and $NR^{19}R^{20}$;

R^{19} and R^{20} are each independently selected from hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl and heterocyclyl;

R^{23} and R^{24} are selected from (i) or (ii) as follows:

(i) R^{23} and R^{24} are independently selected from the group consisting of hydrogen, alkyl, alkenyl, alkynyl, cycloalkyl, aryl and heteroaryl; or

(ii) R^{23} and R^{24} together form alkylene, alkenylene or cycloalkylene;

R^{25}, R^{27} and R^{28} are each independently a monovalent group selected from hydrogen, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy and $NR^{19}R^{20}$;

R^{15}, R^{17}, R^{18}, R^{19}, R^{20}, R^{23}, R^{24}, R^{25}, R^{27} and R^{28} can be substituted with one or more substituents each independently selected from Z^2; Z^2 is selected from alkyl, alkenyl, alkynyl, aryl, cycloalkyl, cycloalkenyl, hydroxy, $S(O)_hR^{35}$; h is 0, 1 or 2, $NR^{35}R^{36}$, $COOR^{35}$, COR^{35}, $CONR^{35}R^{36}$, $OC(O)NR^{35}R^{36}$, $N(R^{35})C(O)R^{36}$, alkoxy, aryloxy, heteroaryl, heterocyclyl, heteroaryloxy, heterocyclyloxy, aralkyl, aralkenyl, aralkynyl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, aralkoxy, heteroaralkoxy, alkoxycarbonyl, carbamoyl, thiocarbamoyl, alkoxycarbonyl, carboxyaryl, halo, pseudohalo, haloalkyl and carboxamido; and

R^{35} and R^{36} are each independently selected from among hydrogen, halo, pseudohalo, cyano, azido, nitro, trialkylsilyl, dialkylarylsilyl, alkyldiarylsilyl, triarylsilyl, alkyl, alkenyl, alkynyl, haloalkyl, haloalkoxy, aryl, aralkyl, aralkenyl, aralkynyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heteroaralkynyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkenyl, heterocyclylalkynyl, hydroxy, alkoxy, aryloxy, aralkoxy, heteroaralkoxy, amino, amido, alkylamino, dialkylamino, alkylarylamino, diarylamino and arylamino.

138. A method of identifying drug non-target biomolecules in a mixture of biomolecules, comprising:

interacting mixture of biomolecules with a collection of capture compounds of claim 1;and

analyzing the captured biomolecules to identify drug non-target.

139. The method of claim 1, wherein X is a photoactivatable group.

140. The method of claim 139, wherein the capture compound interacts with the biomolecule mixture prior to activation of the photoactivatable group.

141. The method of claim 139, wherein the photoactivatable group is an arylazide.

142. The method of claim 139, wherein the photoactivatable group is a phenylazide.

143. A method, comprising:

contacting a capture compound that comprises a drug with a sample containing biomolecules to effect capture of biomolecules in the sample;

isolating and identifying the captured biomolecules; and

re-designing the drug to eliminate or alter its binding interactions with a captured biomolecule.

144. The method of claim 143, further comprising identifying a function of a captured biomolecule.

145. The method of claim 143, wherein the alteration in binding is an increase in binding.

146. The method of claim 143, wherein the alteration in binding is a decrease in binding.

147. The method of claim 143, wherein the biomolecule for which binding is altered is a non-target biomolecule.

148. The method of claim 143, wherein the biolomolecules comprise proteins.

149. The method of claim 143, wherein the sample comprises a body tissue or fluid.

150. The method of claim 143, wherein the capture compound comprises a moiety X that is selected to covalently bind to biomolecules or to bind with sufficiently high affinity so that the resulting complexes of biomolecule/capture compounds are stable under conditions of mass spectrometric analysis; a moiety Y that increases the selectivity of the binding by X such that the capture compound binds to fewer biomlecules when the selectivity moiety is present than in its absence; a moiety Q, wherein Q permits sorting; and a moiety Z for presenting X, Y and Q;

wherein X is latent requiring activation following contacting with the biomolecules to allow for reaction with the biomolecules.

151. The method of claim 143, wherein the sample is contacted with a collection of capture compounds.

152. The method of claim 143, wherein the compound comprises an azide, diazirine or active ester group.

153. The method of claim 143, wherein the method is repeated with the re-designed drug linked to a capture compound to effect further modification thereof.

154. The method of claim 143, wherein the capture compounds bind to the drug at a plurality of sites.

155. The method of claim 143, wherein the captured proteins are drug target proteins.

156. The method of claim 143, wherein the capture proteins are non-drug target proteins.

157. The method of claim 143, wherein the contacting step is performed under conditions whereby the interactions of the drug with proteins in the sample reaches equilibrium.

158. The method claim 157, wherein after equilibrium the mixture is treated to form a covalent bond between the capture agent and the proteins.

159. The method of claim 158, wherein the treatment comprises a change in pH or activation of a capture compound, wherein the capture compound comprises an inert reactivity group prior to activation.

160. The method of claim 143, wherein the concentration of capture compound is varied in a plurality of different reactions.

161. The method of claim 160, wherein a Kd value is determined.

162. The method of claim 143, wherein the structure or identify of the biomolecule is effected by mass spectrometric analysis.

163. The method of claim 162, wherein the mass spectrometry format is selected from among matrix assisted laser desorption ionization (MALDI), continuous or pulsed electrospray (ES) ionization, ionspray, thermospray, and massive cluster impact mass spectrometry.

164. The method of claim 163, wherein the detection format is linear time-of-flight (TOF), reflectron time-of-flight, single quadruple, multiple quadruple, single magnetic sector, multiple magnetic sector, Fourier transform, ion cyclotron resonance (ICR), or ion trap.

165. The method of claim 143, wherein the function of a biomolecule is determined by *in silico, in vitro,* or *in vivo* methods.

166. The method of claim 165, wherein the function of a biomolecule is determined by sequence alignment, pharmacophores, homology models and protein motif correlation, liver midrosomes metabolic pathways, cDNA-expressed enzymes, signal pathways and back-mapping to yeast pathways, simulations and protein/protein interaction of pull-out proteins, native polymorphisms, knock-out/knock-in, flow cytometry, therapeutic activity of the drug, or prospective genotyping and prospective phenotyping

167. The method of claim 143, wherein redesigning the drug results in a second drug with fewer side-effects or an increased therapeutic index as compared to the first drug.

168. The method of claim 143, wherein the drug is selected from among troglitazone, rosiglitazone, pioglitazone, methotrexate, atorvastatin, celecoxib, refecoxib and cerivastatin.